



Author index to volume 197

Al-Kahali, M.S.N., see Lawley, K.P. 197 (1995) 37
Allen, J.P., see Woodbury, N.W. 197 (1995) 405
André, J.-M., see Jacquemin, D. 197 (1995) 107
Aquino, A.J.A., P. Beroza, D.N. Beratan and J.N. Onuchic, Docking and electron transfer between cytochrome c₂ and the photosynthetic reaction center 197 (1995) 277
Ashokkumar, M., see Gauduel, Y. 197 (1995) 167

Baddour-Hadjean, R., F. Filliaux, N. Floquet, S. Belushkin, I. Natkaniec, L. Desgranges and D. Grebille, Inelastic neutron scattering study of proton dynamics in Ca(OH)₂ at 20 K 197 (1995) 81
Baylis, W.E., see Bieroń, J.R. 197 (1995) 129
Belushkin, S., see Baddour-Hadjean, R. 197 (1995) 81
Ben-Nun, M., see Wang, X. 197 (1995) 1
Beratan, D.N., see Aquino, A.J.A. 197 (1995) 277
Beroza, P., see Aquino, A.J.A. 197 (1995) 277
Bieroń, J.R. and W.E. Baylis, Potential energy curves of HgCd and spectroscopic constants of group IIB metal dimers 197 (1995) 129
Bixon, M., J. Jortner and M.E. Michel-Beyerle, A kinetic analysis of the primary charge separation in bacterial photosynthesis. Energy gaps and static heterogeneity 197 (1995) 389
Borowski, P., see Rauk, A. 197 (1995) 73
Boxer, S.G., see Lao, K. 197 (1995) 259
Bruce, J.M., see Labahn, A. 197 (1995) 355
Buntkowsky, G., see Yurkovskaya, A.V. 197 (1995) 157

Champagne, B., see Jacquemin, D. 197 (1995) 107
Chang, H.-C., R. Jankowiak, N.R.S. Reddy and G.J. Small, Pressure dependence of primary charge separation in a photosynthetic reaction center 197 (1995) 307

Desgranges, L., see Baddour-Hadjean, R. 197 (1995) 81
Dézarnaud-Dandine, C. and A. Sevin, A theoretical investigation on the electron-acceptor properties of polar CS bonds of CH_{3-n}F_nSH (*n* = 0–3) thiols and CH_{3-n}F_nSCH_{3-n}F_n (*n* = 0–3) sulfides 197 (1995) 51
Dohle, M., J. Manz, G.K. Paramonov and H. Quast, Design of substituted semibullvalenes suitable for control of the Cope rearrangement by two ps IR laser pulses 197 (1995) 91
Donovan, R.J., see Lawley, K.P. 197 (1995) 37
Dutton, P.L., see Moser, C.C. 197 (1995) 343
Dvinskikh, S.V., see Yurkovskaya, A.V. 197 (1995) 157

Fahr, A., A.K. Nayak and M.J. Kurylo, The ultraviolet absorption cross sections of CH₃I temperature dependent gas and liquid phase measurements 197 (1995) 195

Feher, G., see Labahn, A. 197 (1995) 355
 Fillaux, F., see Baddour-Hadjean, R. 197 (1995) 81
 Fischer, S.F., see Scherer, P.O.J. 197 (1995) 333
 Floquet, N., see Baddour-Hadjean, R. 197 (1995) 81
 Franzen, S., see Lao, K. 197 (1995) 259
 Friese, M., see Hartwich, G. 197 (1995) 423

Gauduel, Y., H. Gelabert and M. Ashokkumar, Short-lived charge-transfer-to-solvent-states and multiple electronic relaxations following femtosecond excitation of aqueous chloride ion 197 (1995) 167
 Gelabert, H., see Gauduel, Y. 197 (1995) 167
 Grebille, D., see Baddour-Hadjean, R. 197 (1995) 81
 Grein, F., see Hachey, M.R.J. 197 (1995) 61
 Gu, X., see Lin, S.H. 197 (1995) 435

Hachey, M.R.J. and F. Grein, The spectroscopy of thioformaldehyde. MR-CI studies on the triplet states of H_2CS 197 (1995) 61
 Hartl, I., see Huber, H. 197 (1995) 297

Hartwich, G., M. Friese, H. Scheer, A. Ogronik and M.E. Michel-Beyerle, Ultrafast internal conversion in $13^2\text{-OH-Ni-bacteriochlorophyll}$ in reaction centers of *Rhodobacter sphaeroides* R26 197 (1995) 423
 Hayashi, M., see Lin, S.H. 197 (1995) 435
 Hochstrasser, R.M., see Moser, C.C. 197 (1995) 343
 Holten, D., see Laporte, L. 197 (1995) 225

Huber, H., M. Meyer, T. Nägele, I. Hartl, H. Scheer, W. Zinth and J. Wachtveitl, Primary photosynthesis in reaction centers containing four different types of electron acceptors at site H_A 197 (1995) 297
 Hush, N.S., see Reimers, J.R. 197 (1995) 323

Ivanov, A.I., V.A. Mikhailova and A.M. Volodin, The effect of magnetic and spin interactions on outer-sphere electron transfer 197 (1995) 19

Jacquemin, D., B. Champagne and J.-M. André, Molecular orbital expressions for approximate uncoupled Hartree-Fock second hyperpolarizabilities. A Pariser-Parr-Pople assessment for model polyacetylene chains 197 (1995) 107
 Jankowiak, R., see Chang, H.-C. 197 (1995) 307
 Jortner, J., see Bixon, M. 197 (1995) 389

Kirmaier, C., see Laporte, L. 197 (1995) 225
 Kurylo, M.J., see Fahr, A. 197 (1995) 195

Labahn, A., J.M. Bruce, M.Y. Okamura and G. Feher, Direct charge recombination from $\text{D}^+\text{Q}_A\text{Q}_B^-$ to $\text{D}\text{Q}_A\text{Q}_B$ in bacterial reaction centers from *Rhodobacter sphaeroides* containing low potential quinone in the Q_A site 197 (1995) 355
 Lambright, D., see Lao, K. 197 (1995) 259
 Lao, K., S. Franzen, M. Steffen, D. Lambright, R. Stanley and S.G. Boxer, Effects of applied electric fields on the quantum yields for the initial electron transfer steps in bacterial photosynthesis. II. Dynamic Stark effect 197 (1995) 259

Laporte, L., C. Kirmaier, C.C. Schenck and D. Holten, Free-energy dependence of the rate of electron transfer to the primary quinone in beta-type reaction centers	197 (1995) 225
Lawley, K.P., T. Ridley, Z. Min, P.J. Wilson, M.S.N. Al-Kahali and R.J. Donovan, Vibronic coupling between Rydberg and ion-pair states of I ₂ investigated by (2 + 1) resonance enhanced multiphoton ionization spectroscopy	197 (1995) 37
Levine, R.D., see Wang, X.	197 (1995) 1
Lin, S., see Woodbury, N.W.	197 (1995) 405
Lin, S.H., M. Hayashi, S. Suzuki, X. Gu, W. Xiao and M. Sugawara, Theoretical analyses on femtosecond time-resolved spectra of initial electron transfer of photosynthetic reaction centers at low temperatures	197 (1995) 435
Lin, X., see Woodbury, N.W.	197 (1995) 405
Malzahn, D. and V. May, Guided motion in a dissipative quantum system: vibrational state preparation using picosecond infrared pulses	197 (1995) 205
Manz, J., see Dohle, M.	197 (1995) 91
May, V., see Malzahn, D.	197 (1995) 205
Meyer, M., see Huber, H.	197 (1995) 297
Michel-Beyerle, M.E., see Bixon, M.	197 (1995) 389
Michel-Beyerle, M.E., see Hartwich, G.	197 (1995) 423
Mikhailova, V.A., see Ivanov, A.I.	197 (1995) 19
Min, Z., see Lawley, K.P.	197 (1995) 37
Möbius, K., see Plato, M.	197 (1995) 289
Morozova, O.B., see Yurkovskaya, A.V.	197 (1995) 157
Moser, C.C., R.J. Sension, A.Z. Szarka, S.T. Repinec, R.M. Hochstrasser and P.L. Dutton, Initial charge separation kinetics of bacterial photosynthetic reaction centers in oriented Langmuir–Blodgett films in an applied electric field	197 (1995) 343
Mukamel, S., see Skourtis, S.S.	197 (1995) 367
Nägele, T., see Huber, H.	197 (1995) 297
Natkaniec, I., see Baddour-Hadjean, R.	197 (1995) 81
Nayak, A.K., see Fahr, A.	197 (1995) 195
Nobusada, K. and K. Sakimoto, A quantum mechanical study of dissociative He + H ₂ collisions	197 (1995) 147
Ogrodnik, A., see Hartwich, G.	197 (1995) 423
Okamura, M.Y., see Labahn, A.	197 (1995) 355
Onuchic, J.N., see Aquino, A.J.A.	197 (1995) 277
Otto, F., E. Tränkle and C. von Borczyskowski, Simulation of exciton transport in binary molecular crystals and comparison with experiments in chemically mixed crystals	197 (1995) 139
Paramonov, G.K., see Dohle, M.	197 (1995) 91
Peloquin, J.M., see Woodbury, N.W.	197 (1995) 405
Plato, M. and K. Möbius, Structural characterization of the primary donor in photosynthetic bacteria by its electronic g-tensor	197 (1995) 289
Quast, H., see Dohle, M.	197 (1995) 91
Rauk, A., D. Yu, P. Borowski and B. Roos, CASSCF, CASPT2, and MRCl investigations of formyloxy radical (HCOO [·])	197 (1995) 73

Reddy, N.R.S., see Chang, H.-C. 197 (1995) 307

Reimers, J.R. and N.S. Hush, Nature of the ground and first excited states of the radical cations of photosynthetic bacterial reaction centres 197 (1995) 323

Repinec, S.T., see Moser, C.C. 197 (1995) 343

Ridley, T., see Lawley, K.P. 197 (1995) 37

Roos, B., see Rauk, A. 197 (1995) 73

Sagdeev, R.Z., see Yurkovskaya, A.V. 197 (1995) 157

Sakimoto, K., see Nobusada, K. 197 (1995) 147

Scharnagl, C., see Scherer, P.O.J. 197 (1995) 333

Scheer, H., see Hartwich, G. 197 (1995) 423

Scheer, H., see Huber, H. 197 (1995) 297

Schenck, C.C., see Laporte, L. 197 (1995) 225

Scherer, P.O.J., C. Scharnagl and S.F. Fischer, Symmetry breakage in the electronic structure of bacterial reaction centers 197 (1995) 333

Sension, R.J., see Moser, C.C. 197 (1995) 343

Sevin, A., see Dézarnaud-Dandine, C. 197 (1995) 51

Skourtis, S.S. and S. Mukamel, Superexchange versus sequential long range electron transfer; density matrix pathways in Liouville space 197 (1995) 367

Small, G.J., On the validity of the standard model for primary charge separation in the bacterial reaction center 197 (1995) 239

Small, G.J., see Chang, H.-C. 197 (1995) 307

Stanley, R., see Lao, K. 197 (1995) 259

Steer, R.P., see Tittelbach-Helmrich, D. 197 (1995) 99

Steffen, M., see Lao, K. 197 (1995) 259

Sugawara, M., see Lin, S.H. 197 (1995) 435

Suzuki, S., see Lin, S.H. 197 (1995) 435

Szarka, A.Z., see Moser, C.C. 197 (1995) 343

Taguchi, A.K.W., see Woodbury, N.W. 197 (1995) 405

Tittelbach-Helmrich, D. and R.P. Steer, Measurements of the subpicosecond relaxation rates of the first excited singlet states of some pseudoazulenes in solution 197 (1995) 99

Tränkle, E., see Otto, F. 197 (1995) 139

Vieth, H.-M., see Yurkovskaya, A.V. 197 (1995) 157

Volodin, A.M., see Ivanov, A.I. 197 (1995) 19

von Borczyskowski, C., see Otto, F. 197 (1995) 139

Wachtveitl, J., see Huber, H. 197 (1995) 297

Wang, X., M. Ben-Nun and R.D. Levine, Peripheral dynamics of the $\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3$ reaction. A classical trajectory computation 197 (1995) 1

Williams, J.A.C., see Woodbury, N.W. 197 (1995) 405

Wilson, P.J., see Lawley, K.P. 197 (1995) 37

Woodbury, N.W., S. Lin, X. Lin, J.M. Peloquin, A.K.W. Taguchi, J.A.C. Williams and J.P. Allen, The role of reaction center excited state evolution during charge separation in a *Rb. sphaeroides* mutant with an initial electron donor midpoint potential 260 mV above wild type 197 (1995) 405

Xiao, W., see Lin, S.H. 197 (1995) 435

Yu, D., see Rauk, A. 197 (1995) 73

Yurkovskaya, A.V., O.B. Morozova, R.Z. Sagdeev, S.V. Dvinskikh, G. Buntkowsky and H.-M. Vieth, The influence of scavenging on CIDNP field dependences in biradicals during the photolysis of large-ring cycloalkanones 197 (1995) 157

Zinth, W., see Huber, H. 197 (1995) 297



Subject index to volume 197

Methods

Theoretical

Classical mechanics

Peripheral dynamics of the $\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3$ reaction. A classical trajectory computation, X. Wang, M. Ben-Nun and R.D. Levine

197 (1995) 1

Many body and quasiparticle approaches

The effect of magnetic and spin interactions on outer-sphere electron transfer, A.I. Ivanov, V.A. Mikhailova and A.M. Volodin

197 (1995) 19

Coupling schemes and perturbative treatments

Vibronic coupling between Rydberg and ion-pair states of I_2 investigated by (2 + 1) resonance enhanced multiphoton ionization spectroscopy, K.P. Lawley, T. Ridley, Z. Min, P.J. Wilson, M.S.N. Al-Kahali and R.J. Donovan

197 (1995) 37

Molecular orbital expressions for approximate uncoupled Hartree–Fock second hyperpolarizabilities. A Pariser–Parr–Pople assessment for model polyacetylene chains, D. Jacquemin, B. Champagne and J.-M. André

197 (1995) 107

Superexchange versus sequential long range electron transfer; density matrix pathways in Liouville space, S.S. Skourtis and S. Mukamel

197 (1995) 367

A kinetic analysis of the primary charge separation in bacterial photosynthesis. Energy gaps and static heterogeneity, M. Bixon, J. Jortner and M.E. Michel-Beyerle

197 (1995) 389

Theoretical analyses on femtosecond time-resolved spectra of initial electron transfer of photosynthetic reaction centers at low temperatures, S.H. Lin, M. Hayashi, S. Suzuki, X. Gu, W. Xiao and M. Sugawara

197 (1995) 435

Transport quantum mechanics

Guided motion in a dissipative quantum system: vibrational state preparation using picosecond infrared pulses, D. Malzahn and V. May

197 (1995) 205

Superexchange versus sequential long range electron transfer; density matrix pathways in Liouville space, S.S. Skourtis and S. Mukamel

197 (1995) 367

Ab initio schemes for stationary properties

A theoretical investigation on the electron–acceptor properties of polar CS bonds of $\text{CH}_{3-n}\text{F}_n\text{SH}$ ($n = 0–3$) thiols and $\text{CH}_{3-n}\text{F}_n\text{SCH}_{3-n}\text{F}_n$ ($n = 0–3$) sulfides, C. Dézarnaud-Dandine and A. Sevin

197 (1995) 51

The spectroscopy of thioformaldehyde. MR-CI studies on the triplet states of H_2CS , M.R.J. Hachey and F. Grein

197 (1995) 61

CASSCF, CASPT2, and MRCI investigations of formyloxyl radical (HCOO^\cdot), A. Rauk, D. Yu, P. Borowski and B. Roos	197 (1995) 73
Potential energy curves of HgCd and spectroscopic constants of group IIB metal dimers, J.R. Bieroń and W.E. Baylis	197 (1995) 129
 <i>Computational and simulation methods</i>	
Simulation of exciton transport in binary molecular crystals and comparison with experiments in chemically mixed crystals, F. Otto, E. Tränkle and C. von Borczyskowski	197 (1995) 139
Docking and electron transfer between cytochrome c_2 and the photosynthetic reaction center, A.J.A. Aquino, P. Beroza, D.N. Beratan and J.N. Onuchic	197 (1995) 277
Nature of the ground and first excited states of the radical cations of photosynthetic bacterial reaction centres, J.R. Reimers and N.S. Hush	197 (1995) 323
Symmetry breakage in the electronic structure of bacterial reaction centers, P.O.J. Scherer, C. Scharnagl and S.F. Fischer	197 (1995) 333
 <i>Molecular dynamics and scattering theory</i>	
Peripheral dynamics of the $\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3$ reaction. A classical trajectory computation, X. Wang, M. Ben-Nun and R.D. Levine	197 (1995) 1
Inelastic neutron scattering study of proton dynamics in Ca(OH)_2 at 20 K, R. Baddour-Hadjean, F. Filliaux, N. Floquet, S. Belushkin, I. Natkaniec, L. Desgranges and D. Grebille	197 (1995) 81
Design of substituted semibullvalenes suitable for control of the Cope rearrangement by two ps IR laser pulses, M. Dohle, J. Manz, G.K. Paramonov and H. Quast	197 (1995) 91
A quantum mechanical study of dissociative $\text{He} + \text{H}_2$ collisions, K. Nobusada and K. Sakimoto	197 (1995) 147
 Experimental	
 <i>Magnetic resonances</i>	
The influence of scavenging on CIDNP field dependences in biradicals during the photolysis of large-ring cycloalkanones, A.V. Yurkovskaya, O.B. Morozova, R.Z. Sagdeev, S.V. Dvinskikh, G. Bunkowsky and H.-M. Vieth	197 (1995) 157
Structural characterization of the primary donor in photosynthetic bacteria by its electronic g -tensor, M. Plato and K. Möbius	197 (1995) 289
 <i>Infrared spectroscopy</i>	
Inelastic neutron scattering study of proton dynamics in Ca(OH)_2 at 20 K, R. Baddour-Hadjean, F. Filliaux, N. Floquet, S. Belushkin, I. Natkaniec, L. Desgranges and D. Grebille	197 (1995) 81
Short-lived charge-transfer-to-solvent-states and multiple electronic relaxations following femtosecond excitation of aqueous chloride ion, Y. Gauduel, H. Gelabert and M. Ashokkumar	197 (1995) 167
 <i>Raman spectroscopy</i>	
Inelastic neutron scattering study of proton dynamics in Ca(OH)_2 at 20 K, R. Baddour-Hadjean, F. Filliaux, N. Floquet, S. Belushkin, I. Natkaniec, L. Desgranges and D. Grebille	197 (1995) 81

Visible and UV spectroscopy

Vibronic coupling between Rydberg and ion-pair states of I₂ investigated by (2 + 1) resonance enhanced multiphoton ionization spectroscopy, K.P. Lawley, T. Ridley, Z. Min, P.J. Wilson, M.S.N. Al-Kahali and R.J. Donovan 197 (1995) 37

The ultraviolet absorption cross sections of CH₃I temperature dependent gas and liquid phase measurements, A. Fahr, A.K. Nayak and M.J. Kurylo 197 (1995) 195

On the validity of the standard model for primary charge separation in the bacterial reaction center, G.J. Small 197 (1995) 239

Effects of applied electric fields on the quantum yields for the initial electron transfer steps in bacterial photosynthesis. II. Dynamic Stark effect, K. Lao, S. Franzen, M. Steffen, D. Lambright, R. Stanley and S.G. Boxer 197 (1995) 259

Pressure dependence of primary charge separation in a photosynthetic reaction center, H.-C. Chang, R. Jankowiak, N.R.S. Reddy and G.J. Small 197 (1995) 307

Initial charge separation kinetics of bacterial photosynthetic reaction centers in oriented Langmuir-Blodgett films in an applied electric field, C.C. Moser, R.J. Sension, A.Z. Szarka, S.T. Repinec, R.M. Hochstrasser and P.L. Dutton 197 (1995) 343

Direct charge recombination from D⁺Q_AQ_B⁻ to DQ_AQ_B in bacterial reaction centers from *Rhodobacter sphaeroides* containing low potential quinone in the Q_A site, A. Labahn, J.M. Bruce, M.Y. Okamura and G. Feher 197 (1995) 355

Ultrafast internal conversion in 13²-OH-Ni-bacteriochlorophyll in reaction centers of *Rhodobacter sphaeroides* R26, G. Hartwich, M. Friese, H. Scheer, A. Ogrodnik and M.E. Michel-Beyerle 197 (1995) 423

Fluorescence spectroscopy

Ultrafast internal conversion in 13²-OH-Ni-bacteriochlorophyll in reaction centers of *Rhodobacter sphaeroides* R26, G. Hartwich, M. Friese, H. Scheer, A. Ogrodnik and M.E. Michel-Beyerle 197 (1995) 423

Laser methods

Design of substituted semibullvalenes suitable for control of the Cope rearrangement by two ps IR laser pulses, M. Dohle, J. Manz, G.K. Paramonov and H. Quast 197 (1995) 91

Pressure dependence of primary charge separation in a photosynthetic reaction center, H.-C. Chang, R. Jankowiak, N.R.S. Reddy and G.J. Small 197 (1995) 307

Picosecond spectroscopy

Measurements of the subpicosecond relaxation rates of the first excited singlet states of some pseudoazulenes in solution, D. Tittelbach-Helmrich and R.P. Steer 197 (1995) 99

Free-energy dependence of the rate of electron transfer to the primary quinone in beta-type reaction centers, L. Laporte, C. Kirmaier, C.C. Schenck and D. Holten 197 (1995) 225

Primary photosynthesis in reaction centers containing four different types of electron acceptors at site H_A, H. Huber, M. Meyer, T. Nägele, I. Hartl, H. Scheer, W. Zinth and J. Wachtveitl 197 (1995) 297

Initial charge separation kinetics of bacterial photosynthetic reaction centers in oriented Langmuir-Blodgett films in an applied electric field, C.C. Moser, R.J. Sension, A.Z. Szarka, S.T. Repinec, R.M. Hochstrasser and P.L. Dutton 197 (1995) 343

The role of reaction center excited state evolution during charge separation in a *Rb. sphaeroides* mutant with an initial electron donor midpoint potential 260 mV above wild type, N.W. Woodbury, S. Lin, X. Lin, J.M. Peloquin, A.K.W. Taguchi, J.A.C. Williams and J.P. Allen 197 (1995) 405

Non-linear optical spectroscopy

On the validity of the standard model for primary charge separation in the bacterial reaction center, G.J. Small

197 (1995) 239

Optical pumping

Design of substituted semibullvalenes suitable for control of the Cope rearrangement by two ps IR laser pulses, M. Dohle, J. Manz, G.K. Paramonov and H. Quast

197 (1995) 91

Time-resolved experiments

Short-lived charge-transfer-to-solvent-states and multiple electronic relaxations following femtosecond excitation of aqueous chloride ion, Y. Gauduel, H. Gelabert and M. Ashokkumar

197 (1995) 167

Initial charge separation kinetics of bacterial photosynthetic reaction centers in oriented Langmuir-Blodgett films in an applied electric field, C.C. Moser, R.J. Sension, A.Z. Szarka, S.T. Repinec, R.M. Hochstrasser and P.L. Dutton

197 (1995) 343

Direct charge recombination from $D^+Q_AQ_B^-$ to DQ_AQ_B in bacterial reaction centers from *Rhodobacter sphaeroides* containing low potential quinone in the Q_A site, A. Labahn, J.M. Bruce, M.Y. Okamura and G. Feher

197 (1995) 355

The role of reaction center excited state evolution during charge separation in a *Rb. sphaeroides* mutant with an initial electron donor midpoint potential 260 mV above wild type, N.W. Woodbury, S. Lin, X. Lin, J.M. Peloquin, A.K.W. Taguchi, J.A.C. Williams and J.P. Allen

197 (1995) 405

Neutron scattering

Inelastic neutron scattering study of proton dynamics in $\text{Ca}(\text{OH})_2$ at 20 K, R. Baddour-Hadjean, F. Filliaux, N. Floquet, S. Belushkin, I. Natkaniec, L. Desgranges and D. Grebille

197 (1995) 81

Objects**Bulk systems***Gases*

Vibronic coupling between Rydberg and ion-pair states of I_2 investigated by (2 + 1) resonance enhanced multiphoton ionization spectroscopy, K.P. Lawley, T. Ridley, Z. Min, P.J. Wilson, M.S.N. Al-Kahali and R.J. Donovan

197 (1995) 37

The spectroscopy of thioformaldehyde. MR-CI studies on the triplet states of H_2CS , M.R.J. Hachey and F. Grein

197 (1995) 61

The ultraviolet absorption cross sections of CH_3I temperature dependent gas and liquid phase measurements, A. Fahr, A.K. Nayak and M.J. Kurylo

197 (1995) 195

Liquid mixtures and solutions

Short-lived charge-transfer-to-solvent-states and multiple electronic relaxations following femtosecond excitation of aqueous chloride ion, Y. Gauduel, H. Gelabert and M. Ashokkumar

197 (1995) 167

*Crystals**-mixed*

Simulation of exciton transport in binary molecular crystals and comparison with experiments in chemically mixed crystals, F. Otto, E. Tränkle and C. von Borczyskowski

197 (1995) 139

Polymers

Molecular orbital expressions for approximate uncoupled Hartree–Fock second hyperpolarizabilities. A Pariser–Parr–Pople assessment for model polyacetylene chains, D. Jacquemin, B. Champagne and J.-M. André

197 (1995) 107

Biological systems

Free-energy dependence of the rate of electron transfer to the primary quinone in beta-type reaction centers, L. Laporte, C. Kirmaier, C.C. Schenck and D. Holten

197 (1995) 225

On the validity of the standard model for primary charge separation in the bacterial reaction center, G.J. Small

197 (1995) 239

Effects of applied electric fields on the quantum yields for the initial electron transfer steps in bacterial photosynthesis. II. Dynamic Stark effect, K. Lao, S. Franzen, M. Steffen, D. Lambright, R. Stanley and S.G. Boxer

197 (1995) 259

Docking and electron transfer between cytochrome c_2 and the photosynthetic reaction center, A.J.A. Aquino, P. Beroza, D.N. Beratan and J.N. Onuchic

197 (1995) 277

Primary photosynthesis in reaction centers containing four different types of electron acceptors at site H_A , H. Huber, M. Meyer, T. Nägele, I. Hartl, H. Scheer, W. Zinth and J. Wachtveitl

197 (1995) 297

Pressure dependence of primary charge separation in a photosynthetic reaction center, H.-C. Chang, R. Jankowiak, N.R.S. Reddy and G.J. Small

197 (1995) 307

Initial charge separation kinetics of bacterial photosynthetic reaction centers in oriented Langmuir–Blodgett films in an applied electric field, C.C. Moser, R.J. Sension, A.Z. Szarka, S.T. Repinec, R.M. Hochstrasser and P.L. Dutton

197 (1995) 343

Direct charge recombination from $D^+Q_AQ_B^-$ to DQ_AQ_B in bacterial reaction centers from *Rhodobacter sphaeroides* containing low potential quinone in the Q_A site, A. Labahn, J.M. Bruce, M.Y. Okamura and G. Feher

197 (1995) 355

Superexchange versus sequential long range electron transfer; density matrix pathways in Liouville space, S.S. Skourtis and S. Mukamel

197 (1995) 367

A kinetic analysis of the primary charge separation in bacterial photosynthesis. Energy gaps and static heterogeneity, M. Bixon, J. Jortner and M.E. Michel-Beyerle

197 (1995) 389

The role of reaction center excited state evolution during charge separation in a *Rb. sphaeroides* mutant with an initial electron donor midpoint potential 260 mV above wild type, N.W. Woodbury, S. Lin, X. Lin, J.M. Peloquin, A.K.W. Taguchi, J.A.C. Williams and J.P. Allen

197 (1995) 405

Theoretical analyses on femtosecond time-resolved spectra of initial electron transfer of photosynthetic reaction centers at low temperatures, S.H. Lin, M. Hayashi, S. Suzuki, X. Gu, W. Xiao and M. Sugawara

197 (1995) 435

Ultrafast internal conversion in $13^2\text{-OH-Ni-bacteriochlorophyll}$ in reaction centers of *Rhodobacter sphaeroides* R26, G. Hartwich, M. Friese, H. Scheer, A. Ogrodnik and M.E. Michel-Beyerle

197 (1995) 423

Microscopic systems**Molecules (neutral and ionic)**

Peripheral dynamics of the $\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3$ reaction. A classical trajectory computation, X. Wang, M. Ben-Nun and R.D. Levine

197 (1995) 1

The ultraviolet absorption cross sections of CH_3I temperature dependent gas and liquid phase measurements, A. Fahr, A.K. Nayak and M.J. Kurylo 197 (1995) 195

Superexchange versus sequential long range electron transfer; density matrix pathways in Liouville space, S.S. Skourtis and S. Mukamel 197 (1995) 367

-diatomic

Vibronic coupling between Rydberg and ion-pair states of I_2 investigated by (2 + 1) resonance enhanced multiphoton ionization spectroscopy, K.P. Lawley, T. Ridley, Z. Min, P.J. Wilson, M.S.N. Al-Kahali and R.J. Donovan 197 (1995) 37

Potential energy curves of HgCd and spectroscopic constants of group IIB metal dimers, J.R. Bieroń and W.E. Baylis 197 (1995) 129

A quantum mechanical study of dissociative $\text{He} + \text{H}_2$ collisions, K. Nobusada and K. Sakimoto 197 (1995) 147

-small polyatomics

A theoretical investigation on the electron-acceptor properties of polar CS bonds of $\text{CH}_{3-n}\text{F}_n\text{SH}$ ($n = 0-3$) thiols and $\text{CH}_{3-n}\text{F}_n\text{SCH}_{3-n}\text{F}_n$ ($n = 0-3$) sulfides, C. Dézarnaud-Dandine and A. Sevin 197 (1995) 51

The spectroscopy of thioformaldehyde. MR-CI studies on the triplet states of H_2CS , M.R.J. Hachey and F. Grein 197 (1995) 61

-other large

Design of substituted semibullvalenes suitable for control of the Cope rearrangement by two ps IR laser pulses, M. Dohle, J. Manz, G.K. Paramonov and H. Quast 197 (1995) 91

-polymeric and biological

Docking and electron transfer between cytochrome c_2 and the photosynthetic reaction center, A.J.A. Aquino, P. Beroza, D.N. Beratan and J.N. Onuchic 197 (1995) 277

Structural characterization of the primary donor in photosynthetic bacteria by its electronic g-tensor, M. Plato and K. Möbius 197 (1995) 289

Symmetry breakage in the electronic structure of bacterial reaction centers, P.O.J. Scherer, C. Scharnagl and S.F. Fischer 197 (1995) 333

A kinetic analysis of the primary charge separation in bacterial photosynthesis. Energy gaps and static heterogeneity, M. Bixon, J. Jortner and M.E. Michel-Beyerle 197 (1995) 389

Theoretical analyses on femtosecond time-resolved spectra of initial electron transfer of photosynthetic reaction centers at low temperatures, S.H. Lin, M. Hayashi, S. Suzuki, X. Gu, W. Xiao and M. Sugawara 197 (1995) 435

Molecular aggregates

-dimers

Structural characterization of the primary donor in photosynthetic bacteria by its electronic g-tensor, M. Plato and K. Möbius 197 (1995) 289

Nature of the ground and first excited states of the radical cations of photosynthetic bacterial reaction centres, J.R. Reimers and N.S. Hush 197 (1995) 323

Free radicals (including hydronium and muonium)

A theoretical investigation on the electron-acceptor properties of polar CS bonds of $\text{CH}_{3-n}\text{F}_n\text{SH}$ ($n = 0-3$) thiols and $\text{CH}_{3-n}\text{F}_n\text{SCH}_{3-n}\text{F}_n$ ($n = 0-3$) sulfides, C. Dézarnaud-Dandine and A. Sevin 197 (1995) 51

CASSCF, CASPT2, and MRCI investigations of formyloxyl radical (HCOO^{\cdot}), A. Rauk, D. Yu, P. Borowski and B. Roos

197 (1995) 73

The influence of scavenging on CIDNP field dependences in biradicals during the photolysis of large-ring cycloalkanones, A.V. Yurkovskaya, O.B. Morozova, R.Z. Sagdeev, S.V. Dvinskikh, G. Buntkowsky and H.-M. Vieth

197 (1995) 157

Phenomena

Molecular structure

CASSCF, CASPT2, and MRCI investigations of formyloxyl radical (HCOO^{\cdot}), A. Rauk, D.

Yu, P. Borowski and B. Roos

197 (1995) 73

Design of substituted semibullvalenes suitable for control of the Cope rearrangement by two ps IR laser pulses, M. Dohle, J. Manz, G.K. Paramonov and H. Quast

197 (1995) 91

Structural characterization of the primary donor in photosynthetic bacteria by its electronic *g*-tensor, M. Plato and K. Möbius

197 (1995) 289

Vibrations and rotations of molecules

The spectroscopy of thioformaldehyde. MR-CI studies on the triplet states of H_2CS , M.R.J.

Hachey and F. Grein

197 (1995) 61

Inelastic neutron scattering study of proton dynamics in $\text{Ca}(\text{OH})_2$ at 20 K, R. Baddour-Hadjean, F. Fillaux, N. Floquet, S. Belushkin, I. Natkaniec, L. Desgranges and D. Grebille

197 (1995) 81

Electronic structure and states

A theoretical investigation on the electron-acceptor properties of polar CS bonds of $\text{CH}_{3-n}\text{F}_n\text{SH}$ ($n = 0-3$) thiols and $\text{CH}_{3-n}\text{F}_n\text{SCH}_{3-n}\text{F}_n$ ($n = 0-3$) sulfides, C. Dézarnaud-Dandine and A. Sevin

197 (1995) 51

The spectroscopy of thioformaldehyde. MR-CI studies on the triplet states of H_2CS , M.R.J. Hachey and F. Grein

197 (1995) 61

Potential energy curves of HgCd and spectroscopic constants of group IIB metal dimers, J.R. Bieroń and W.E. Baylis

197 (1995) 129

Short-lived charge-transfer-to-solvent-states and multiple electronic relaxations following femtosecond excitation of aqueous chloride ion, Y. Gauduel, H. Gelabert and M. Ashokkumar

197 (1995) 167

The ultraviolet absorption cross sections of CH_3I temperature dependent gas and liquid phase measurements, A. Fahr, A.K. Nayak and M.J. Kurylo

197 (1995) 195

On the validity of the standard model for primary charge separation in the bacterial reaction center, G.J. Small

197 (1995) 239

Structural characterization of the primary donor in photosynthetic bacteria by its electronic *g*-tensor, M. Plato and K. Möbius

197 (1995) 289

Pressure dependence of primary charge separation in a photosynthetic reaction center, H.-C. Chang, R. Jankowiak, N.R.S. Reddy and G.J. Small

197 (1995) 307

Electric and magnetic properties

The effect of magnetic and spin interactions on outer-sphere electron transfer, A.I. Ivanov, V.A. Mikhailova and A.M. Volodin

197 (1995) 19

Effects of applied electric fields on the quantum yields for the initial electron transfer steps in bacterial photosynthesis. II. Dynamic Stark effect, K. Lao, S. Franzen, M. Steffen, D. Lambright, R. Stanley and S.G. Boxer

197 (1995) 259

Molecular interactions

Symmetry breakage in the electronic structure of bacterial reaction centers, P.O.J. Scherer,
C. Scharnagl and S.F. Fischer

197 (1995) 333

Spectral bandshapes and intensities

The ultraviolet absorption cross sections of CH_3I temperature dependent gas and liquid
phase measurements, A. Fahr, A.K. Nayak and M.J. Kurylo
Nature of the ground and first excited states of the radical cations of photosynthetic
bacterial reaction centres, J.R. Reimers and N.S. Hush

197 (1995) 195

197 (1995) 323

Coupling of electronic and nuclear motion

Vibronic coupling between Rydberg and ion-pair states of I_2 investigated by (2 + 1)
resonance enhanced multiphoton ionization spectroscopy, K.P. Lawley, T. Ridley, Z.
Min, P.J. Wilson, M.S.N. Al-Kahali and R.J. Donovan
Nature of the ground and first excited states of the radical cations of photosynthetic
bacterial reaction centres, J.R. Reimers and N.S. Hush

197 (1995) 37

197 (1995) 323

Energy transfer processes

Simulation of exciton transport in binary molecular crystals and comparison with experi-
ments in chemically mixed crystals, F. Otto, E. Tränkle and C. von Borczyskowski
Ultrafast internal conversion in $13^2\text{-OH-Ni-bacteriochlorophyll}$ in reaction centers of
Rhodobacter sphaeroides R26, G. Hartwich, M. Friese, H. Scheer, A. Ogrodnik and
M.E. Michel-Beyerle

197 (1995) 139

197 (1995) 423

Molecular photophysical processes

Measurements of the subpicosecond relaxation rates of the first excited singlet states of
some pseudoazulenes in solution, D. Tittelbach-Helmrich and R.P. Steer
Nature of the ground and first excited states of the radical cations of photosynthetic
bacterial reaction centres, J.R. Reimers and N.S. Hush
Symmetry breakage in the electronic structure of bacterial reaction centers, P.O.J. Scherer,
C. Scharnagl and S.F. Fischer
Ultrafast internal conversion in $13^2\text{-OH-Ni-bacteriochlorophyll}$ in reaction centers of
Rhodobacter sphaeroides R26, G. Hartwich, M. Friese, H. Scheer, A. Ogrodnik and
M.E. Michel-Beyerle

197 (1995) 99

197 (1995) 323

197 (1995) 333

197 (1995) 423

Intramolecular dynamics

Peripheral dynamics of the $\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3$ reaction. A classical trajectory compu-
tation, X. Wang, M. Ben-Nun and R.D. Levine
Guided motion in a dissipative quantum system: vibrational state preparation using
picosecond infrared pulses, D. Malzahn and V. May

197 (1995) 1

197 (1995) 205

Non-linear responses (including optical)

Molecular orbital expressions for approximate uncoupled Hartree–Fock second hyperpolar-
izabilities. A Pariser–Parr–Pople assessment for model polyacetylene chains, D.
Jacquemin, B. Champagne and J.-M. André

197 (1995) 107

*Reactions (including dissociation)**-gas phase*

Peripheral dynamics of the $\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3$ reaction. A classical trajectory computation, X. Wang, M. Ben-Nun and R.D. Levine

197 (1995) 1

A quantum mechanical study of dissociative $\text{He} + \text{H}_2$ collisions, K. Nobusada and K. Sakimoto

197 (1995) 147

-photochemical

The influence of scavenging on CIDNP field dependences in biradicals during the photolysis of large-ring cycloalkanones, A.V. Yurkovskaya, O.B. Morozova, R.Z. Sagdeev, S.V. Dvinskikh, G. Bunkowsky and H.-M. Vieth

197 (1995) 157

On the validity of the standard model for primary charge separation in the bacterial reaction center, G.J. Small

197 (1995) 239

The role of reaction center excited state evolution during charge separation in a *Rb. sphaeroides* mutant with an initial electron donor midpoint potential 260 mV above wild type, N.W. Woodbury, S. Lin, X. Lin, J.M. Peloquin, A.K.W. Taguchi, J.A.C. Williams and J.P. Allen

197 (1995) 405

Electron transfer

The effect of magnetic and spin interactions on outer-sphere electron transfer, A.I. Ivanov, V.A. Mikhailova and A.M. Volodin

197 (1995) 19

A theoretical investigation on the electron-acceptor properties of polar CS bonds of $\text{CH}_{3-n}\text{F}_n\text{SH}$ ($n = 0-3$) thiols and $\text{CH}_{3-n}\text{F}_n\text{SCH}_{3-n}\text{F}_n$ ($n = 0-3$) sulfides, C. Dézarnaud-Dandine and A. Sevin

197 (1995) 51

Short-lived charge-transfer-to-solvent-states and multiple electronic relaxations following femtosecond excitation of aqueous chloride ion, Y. Gauduel, H. Gelabert and M. Ashokumar

197 (1995) 167

Free-energy dependence of the rate of electron transfer to the primary quinone in beta-type reaction centers, L. Laporte, C. Kirmaier, C.C. Schenck and D. Holten

197 (1995) 225

Effects of applied electric fields on the quantum yields for the initial electron transfer steps in bacterial photosynthesis. II. Dynamic Stark effect, K. Lao, S. Franzen, M. Steffen, D. Lambright, R. Stanley and S.G. Boxer

197 (1995) 259

Docking and electron transfer between cytochrome c_2 and the photosynthetic reaction center, A.J.A. Aquino, P. Beroza, D.N. Beratan and J.N. Onuchic

197 (1995) 277

Primary photosynthesis in reaction centers containing four different types of electron acceptors at site H_A , H. Huber, M. Meyer, T. Nägele, I. Hartl, H. Scheer, W. Zinth and J. Wachtveitl

197 (1995) 297

Pressure dependence of primary charge separation in a photosynthetic reaction center, H.-C. Chang, R. Jankowiak, N.R.S. Reddy and G.J. Small

197 (1995) 307

Symmetry breakage in the electronic structure of bacterial reaction centers, P.O.J. Scherer, C. Scharnagl and S.F. Fischer

197 (1995) 333

Initial charge separation kinetics of bacterial photosynthetic reaction centers in oriented Langmuir-Blodgett films in an applied electric field, C.C. Moser, R.J. Sension, A.Z. Szarka, S.T. Repinec, R.M. Hochstrasser and P.L. Dutton

197 (1995) 343

Direct charge recombination from $\text{D}^+ \text{Q}_A^- \text{Q}_B^-$ to $\text{DQ}_A^- \text{Q}_B^-$ in bacterial reaction centers from *Rhodobacter sphaeroides* containing low potential quinone in the Q_A site, A. Labahn, J.M. Bruce, M.Y. Okamura and G. Feher

197 (1995) 355

Superexchange versus sequential long range electron transfer; density matrix pathways in Liouville space, S.S. Skourtis and S. Mukamel 197 (1995) 367

A kinetic analysis of the primary charge separation in bacterial photosynthesis. Energy gaps and static heterogeneity, M. Bixon, J. Jortner and M.E. Michel-Beyerle 197 (1995) 389

The role of reaction center excited state evolution during charge separation in a *Rb. sphaeroides* mutant with an initial electron donor midpoint potential 260 mV above wild type, N.W. Woodbury, S. Lin, X. Lin, J.M. Peloquin, A.K.W. Taguchi, J.A.C. Williams and J.P. Allen 197 (1995) 405

Theoretical analyses on femtosecond time-resolved spectra of initial electron transfer of photosynthetic reaction centers at low temperatures, S.H. Lin, M. Hayashi, S. Suzuki, X. Gu, W. Xiao and M. Sugawara 197 (1995) 435

